Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy 1997 vol.53 N4 PART A, pages 553-564

Internal rotation in 1,2-di-(p-bromophenyl)ethane: Infrared spectra and normal coordinate calculations

Stolov A., Katsyuba S., Kamalova D., Remizov A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Infrared (4000-250 cm-1) spectra of 1,2-di-(p-bromophenyl)ethane (DPBPE) in crystalline phase, liquid and solutions have been investigated. Molecular mechanics study was performed in order to reveal stable conformations of DPBPE. Six unequivalent minima on the potential energy surface were found, and the normal coordinate analysis of these rotational isomers has been carried out. The conformer which is present in the most stable crystalline modification is shown to have the p-bromophenyl groups in trans positions, the phenyl rings being nearly orthogonal to the CPh-C-C′-C′Ph plane. The experimental spectra in combination with the normal coordinate analysis show the evidence of at least three more stable conformers in the liquid and solutions. Rotations around both CPh-Caliph and Caliph-C′aliph bonds were found to be responsible for the appearance of these conformers. The approximate assignment of the IR bands to the conformers is given.

Keywords

Crystalline phase, Infrared spectra, Normal coordinate analysis